

School of Chemistry Mass Spectrometry Service

SampleID JF1-172
Sample Description
Analysis Name JF1-172_142768_GE5_01_15401.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact

Source Type ESI **Ion Polarity** Positive

Submitter

Jonathan Fowler

Supervisor

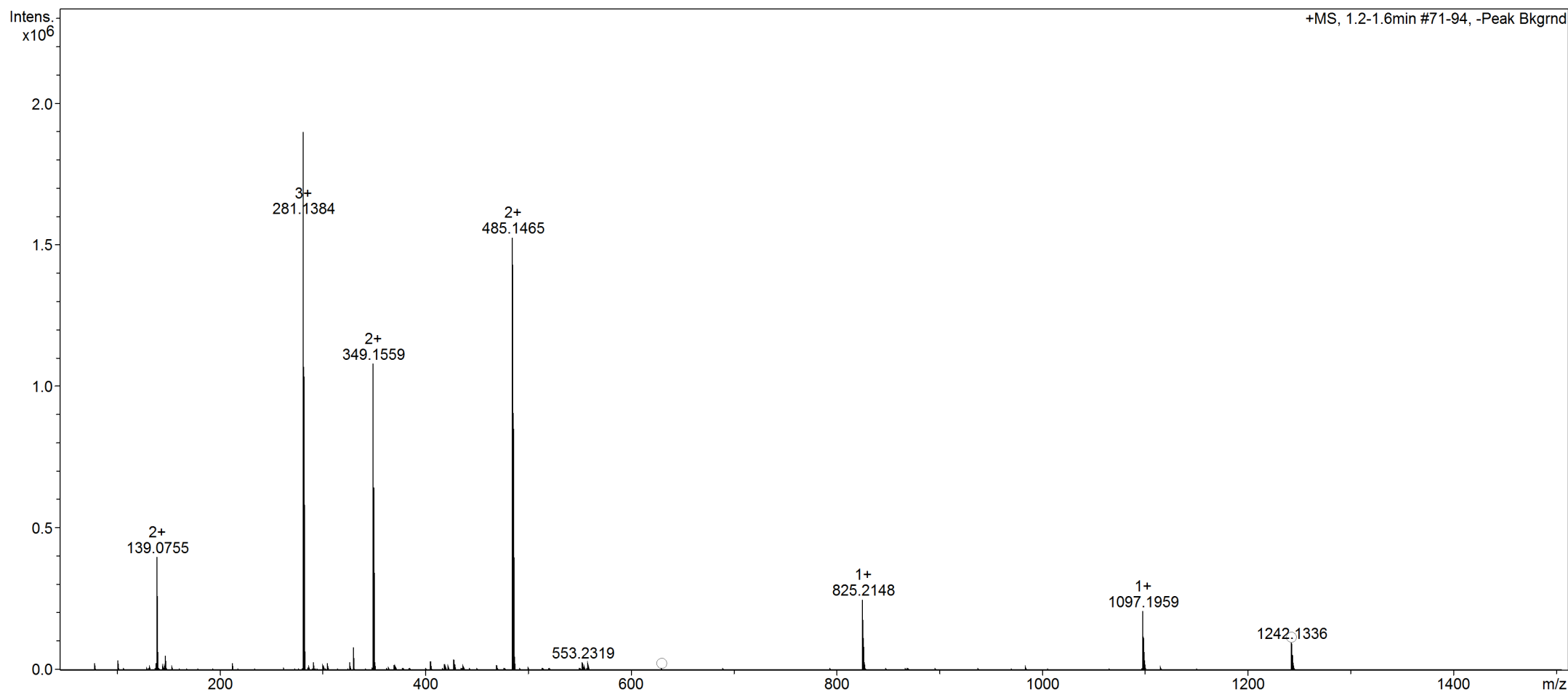
Michaele Hardie

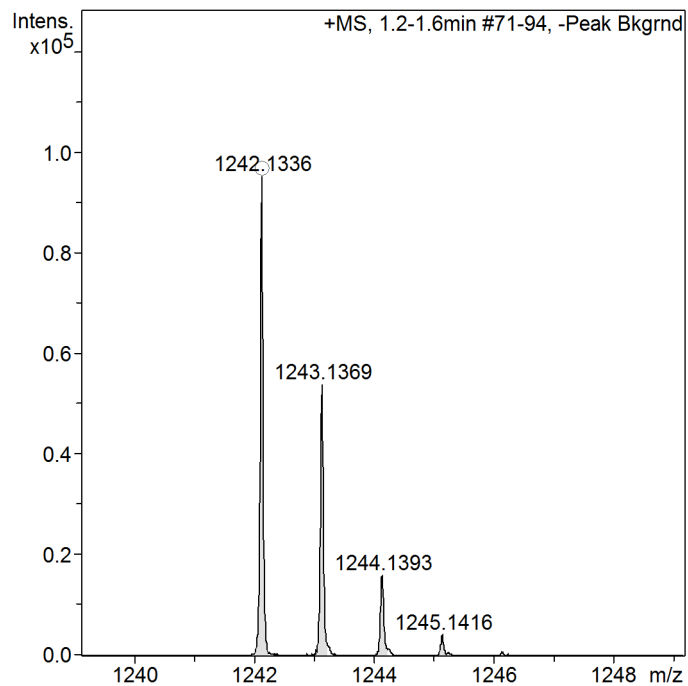
Acquisition Date

16/09/2015 14:24:56

Scan Begin 50 m/z

Scan End 1500 m/z





Confirm/Find Formula Results

The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
630.084125	C51H59I3N8O6	2+	630.084039	0.1	0.1	39.2	100.00	C51 H51 I3 N6 O6	M+NH4
1242.133554	C51H55I3N7O6	1+	1242.134253	0.7	0.6	11.1	100.00		M+NH4

Smart Formula Parameter	Value
Expected Formula	C51H51I3N6O6
Adducts Considered	;M+H;;M+NH4;;M+Na;;M+K;;M+Na 2-H;;2M+H;;2M+Na;

Smart Formula Search Parameters
CHNO and adducts considered
implicitly

Formula Search Minimum	I 6
Formula Search Maximum	

Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	even
Estimate No of Carbons	yes
Filter by H/C Ratio	0 < H/C < 3
Number of Double Bonds & Rings	0 < rings&DB < 80